



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 11:53 AM BST

PDB ID : 6XUB
Title : Structure of coproheme decarboxylase from *Corynebacterium diphtheriae* in complex with monovinyl monopropionyl deuteroheme
Authors : Michlits, H.; Lier, B.; Pfanzagl, V.; Djinovic-Carugo, K.; Furtmueller, P.G.; Oostenbrink, C.; Obinger, C.; Hofbauer, S.
Deposited on : 2020-01-17
Resolution : 1.78 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

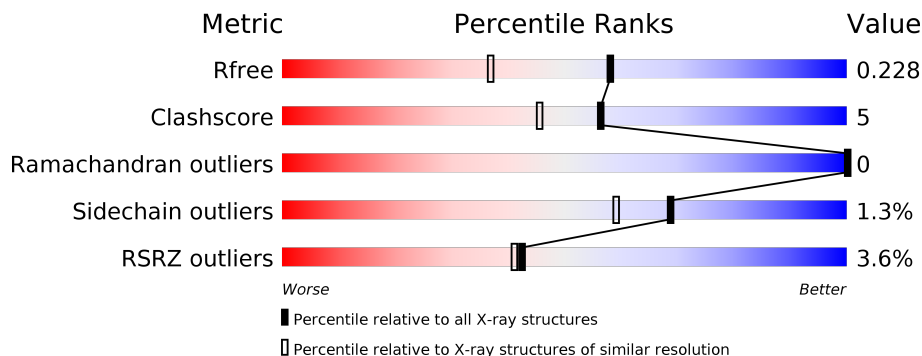
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	
1	B	237	
1	C	237	
1	D	237	
1	E	237	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VOV	A	301	X	-	-	-
2	VOV	B	401	X	-	-	-
2	VOV	C	501	X	-	-	-
2	VOV	D	301	X	-	-	-
2	VOV	E	401	X	-	-	-

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 19489 atoms, of which 9178 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

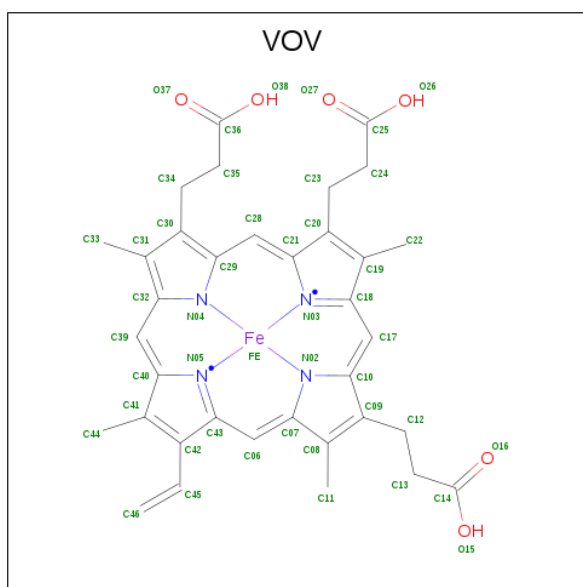
- Molecule 1 is a protein called Chlorite dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	230	3683	1200	1807	330	338	8	0	2	0
1	B	231	3715	1210	1824	332	341	8	0	2	0
1	C	230	3681	1200	1805	330	338	8	0	0	0
1	D	228	3692	1198	1816	332	337	9	0	5	0
1	E	223	3596	1169	1771	322	325	9	0	7	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A2T1BSE4
A	0	PRO	-	expression tag	UNP A0A2T1BSE4
A	235	GLY	-	expression tag	UNP A0A2T1BSE4
B	-1	GLY	-	expression tag	UNP A0A2T1BSE4
B	0	PRO	-	expression tag	UNP A0A2T1BSE4
B	235	GLY	-	expression tag	UNP A0A2T1BSE4
C	-1	GLY	-	expression tag	UNP A0A2T1BSE4
C	0	PRO	-	expression tag	UNP A0A2T1BSE4
C	235	GLY	-	expression tag	UNP A0A2T1BSE4
D	-1	GLY	-	expression tag	UNP A0A2T1BSE4
D	0	PRO	-	expression tag	UNP A0A2T1BSE4
D	235	GLY	-	expression tag	UNP A0A2T1BSE4
E	-1	GLY	-	expression tag	UNP A0A2T1BSE4
E	0	PRO	-	expression tag	UNP A0A2T1BSE4
E	235	GLY	-	expression tag	UNP A0A2T1BSE4

- Molecule 2 is harderoheme (III) (three-letter code: VOV) (formula: $C_{35}H_{34}FeN_4O_6$) (labeled as "Ligand of Interest" by author).

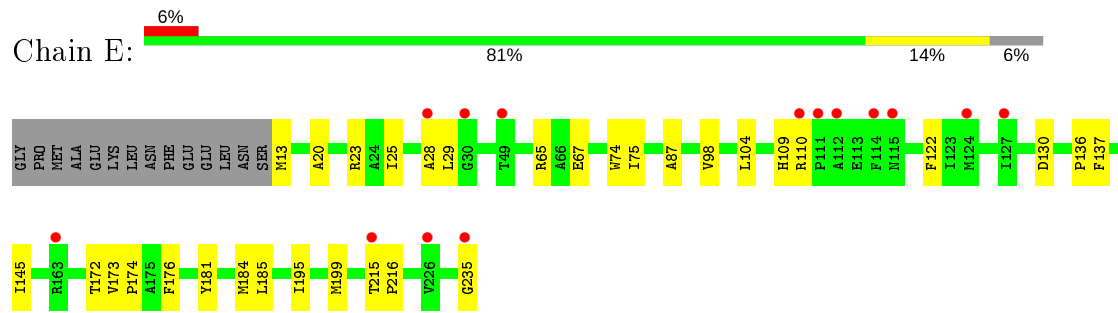


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
2	A	1	77	35	1	31	4	6	0	0
2	B	1	77	35	1	31	4	6	0	0
2	C	1	77	35	1	31	4	6	0	0
2	D	1	77	35	1	31	4	6	0	0
2	E	1	77	35	1	31	4	6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	184	184	184	0	0
3	B	167	167	167	0	0
3	C	164	164	164	0	0
3	D	103	103	103	0	0
3	E	119	119	119	0	0

- Molecule 1: Chlorite dismutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.97Å 123.38Å 78.01Å 90.00° 98.71° 90.00°	Depositor
Resolution (Å)	48.19 – 1.78 48.17 – 1.78	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.19-1.78) 97.9 (48.17-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.78Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.174 , 0.227 0.176 , 0.228	Depositor DCC
R_{free} test set	5272 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtrriage
Anisotropy	0.281	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19489	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VOV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	1/1943 (0.1%)	0.75	1/2631 (0.0%)
1	B	0.55	0/1949	0.68	0/2640
1	C	0.56	1/1927 (0.1%)	0.70	2/2609 (0.1%)
1	D	0.53	0/1945	0.66	1/2631 (0.0%)
1	E	0.51	0/1932	0.67	1/2614 (0.0%)
All	All	0.55	2/9696 (0.0%)	0.69	5/13125 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	MET	SD-CE	-5.43	1.47	1.77
1	C	71	MET	SD-CE	-5.26	1.48	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	13.53	121.84	100.20
1	C	71	MET	CG-SD-CE	10.46	116.93	100.20
1	D	202	MET	CG-SD-CE	6.27	110.24	100.20
1	E	65	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	88	ARG	NE-CZ-NH1	5.38	122.99	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1876	1807	1790	17	0
1	B	1891	1824	1814	12	0
1	C	1876	1805	1805	22	0
1	D	1876	1816	1798	23	1
1	E	1825	1771	1707	22	1
2	A	46	31	0	1	0
2	B	46	31	0	1	0
2	C	46	31	0	0	0
2	D	46	31	0	1	0
2	E	46	31	0	2	0
3	A	184	0	0	6	0
3	B	167	0	0	2	0
3	C	164	0	0	5	0
3	D	103	0	0	5	0
3	E	119	0	0	2	0
All	All	10311	9178	8914	92	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 92 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ARG:NH2	3:D:401:HOH:O	1.72	1.22
1:C:54:GLU:OE2	3:C:601:HOH:O	1.99	0.80
1:D:163:ARG:CZ	3:D:401:HOH:O	2.23	0.77
1:D:163:ARG:NE	1:D:163:ARG:HA	2.01	0.76
1:E:109:HIS:O	3:E:501:HOH:O	2.04	0.75

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ARG:HH22	1:E:130:ASP:OD2 2_756	1.54	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/237 (97%)	225 (98%)	5 (2%)	0	100	100
1	B	231/237 (98%)	228 (99%)	3 (1%)	0	100	100
1	C	228/237 (96%)	224 (98%)	4 (2%)	0	100	100
1	D	231/237 (98%)	224 (97%)	7 (3%)	0	100	100
1	E	228/237 (96%)	220 (96%)	8 (4%)	0	100	100
All	All	1148/1185 (97%)	1121 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/196 (98%)	191 (99%)	2 (1%)	76	68
1	B	194/196 (99%)	191 (98%)	3 (2%)	65	53
1	C	191/196 (97%)	189 (99%)	2 (1%)	76	68
1	D	193/196 (98%)	190 (98%)	3 (2%)	62	51
1	E	191/196 (97%)	189 (99%)	2 (1%)	76	68
All	All	962/980 (98%)	950 (99%)	12 (1%)	69	62

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	74	TRP
1	C	227	SER
1	D	163	ARG
1	B	163	ARG
1	D	74	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	C	6	ASN
1	E	97	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	VOV	B	401	1	28,53,53	0.75	0	18,86,86	1.66	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VOV	C	501	1	28,53,53	0.91	1 (3%)	18,86,86	2.21	8 (44%)
2	VOV	D	301	1	28,53,53	0.89	1 (3%)	18,86,86	2.33	7 (38%)
2	VOV	A	301	1	28,53,53	0.80	0	18,86,86	1.97	6 (33%)
2	VOV	E	401	1	28,53,53	0.96	1 (3%)	18,86,86	1.74	5 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VOV	B	401	1	1/1/9/9	2/9/57/57	-
2	VOV	C	501	1	1/1/9/9	2/9/57/57	-
2	VOV	D	301	1	1/1/9/9	3/9/57/57	-
2	VOV	A	301	1	1/1/9/9	2/9/57/57	-
2	VOV	E	401	1	1/1/9/9	3/9/57/57	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	VOV	C42-C45	2.31	1.52	1.47
2	D	301	VOV	C42-C45	2.26	1.52	1.47
2	C	501	VOV	C42-C45	2.17	1.52	1.47

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	VOV	C35-C34-C30	-5.54	102.27	112.49
2	C	501	VOV	C24-C23-C20	4.76	121.24	112.48
2	A	301	VOV	C42-C43-N05	4.61	115.17	109.21
2	D	301	VOV	C34-C35-C36	3.93	119.27	112.67
2	D	301	VOV	C33-C31-C32	-3.64	122.87	128.46

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	401	VOV	N02
2	C	501	VOV	N02
2	D	301	VOV	N02
2	A	301	VOV	N02

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Mol	Chain	Res	Type	Atom
2	E	401	VOV	N02

5 of 12 torsion outliers are listed below:

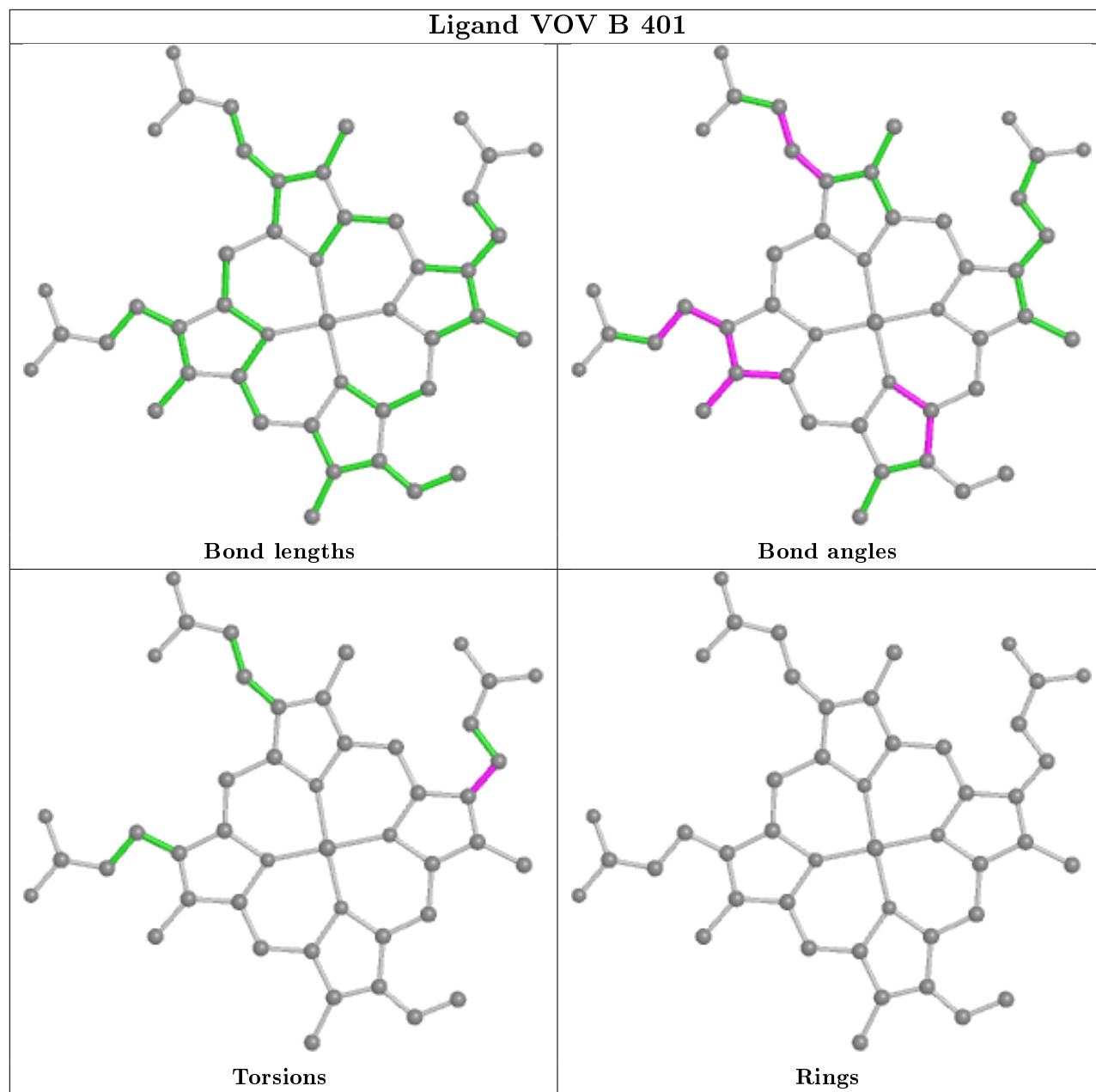
Mol	Chain	Res	Type	Atoms
2	B	401	VOV	C08-C09-C12-C13
2	B	401	VOV	C10-C09-C12-C13
2	D	301	VOV	C08-C09-C12-C13
2	D	301	VOV	C10-C09-C12-C13
2	A	301	VOV	C08-C09-C12-C13

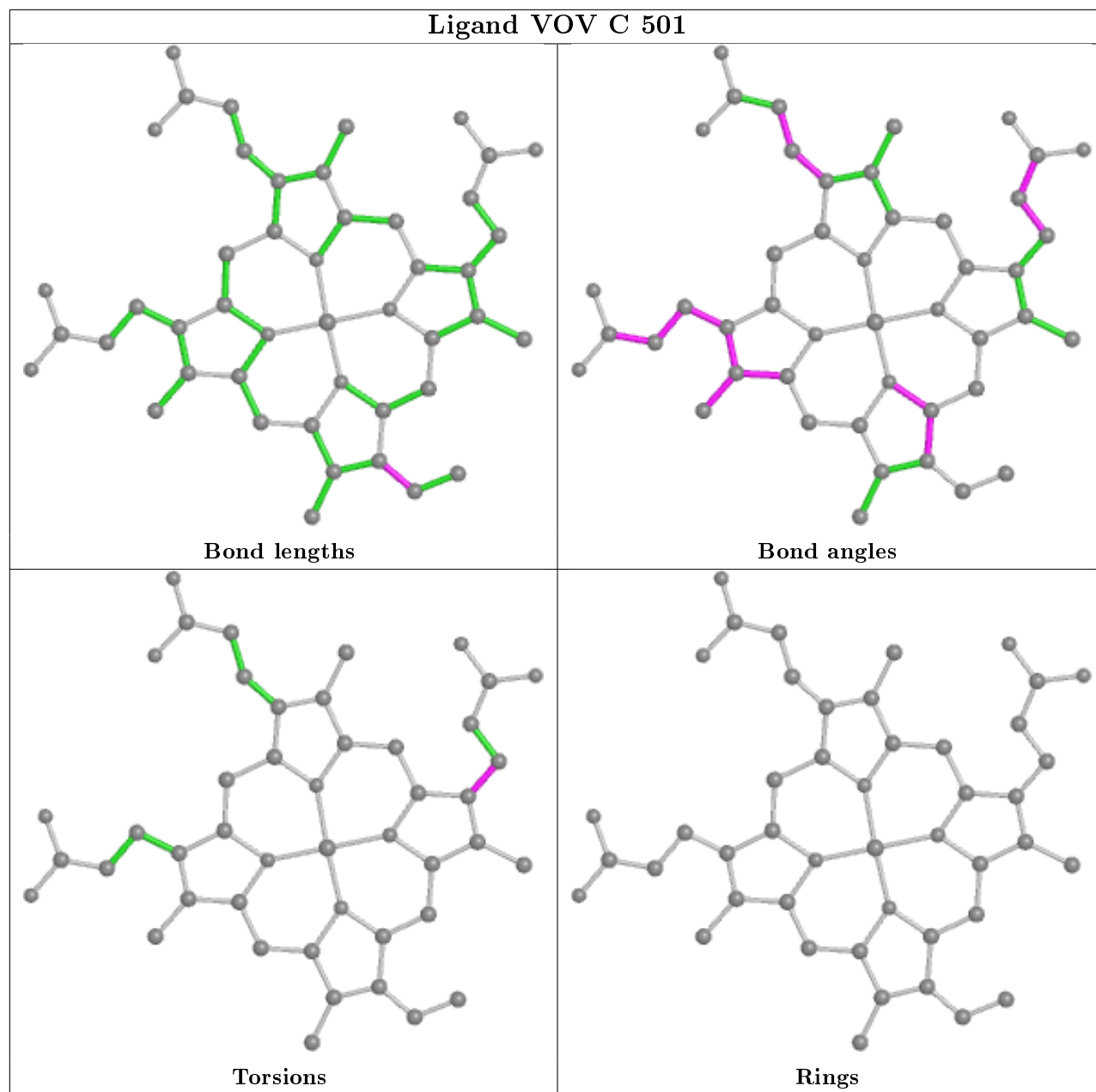
There are no ring outliers.

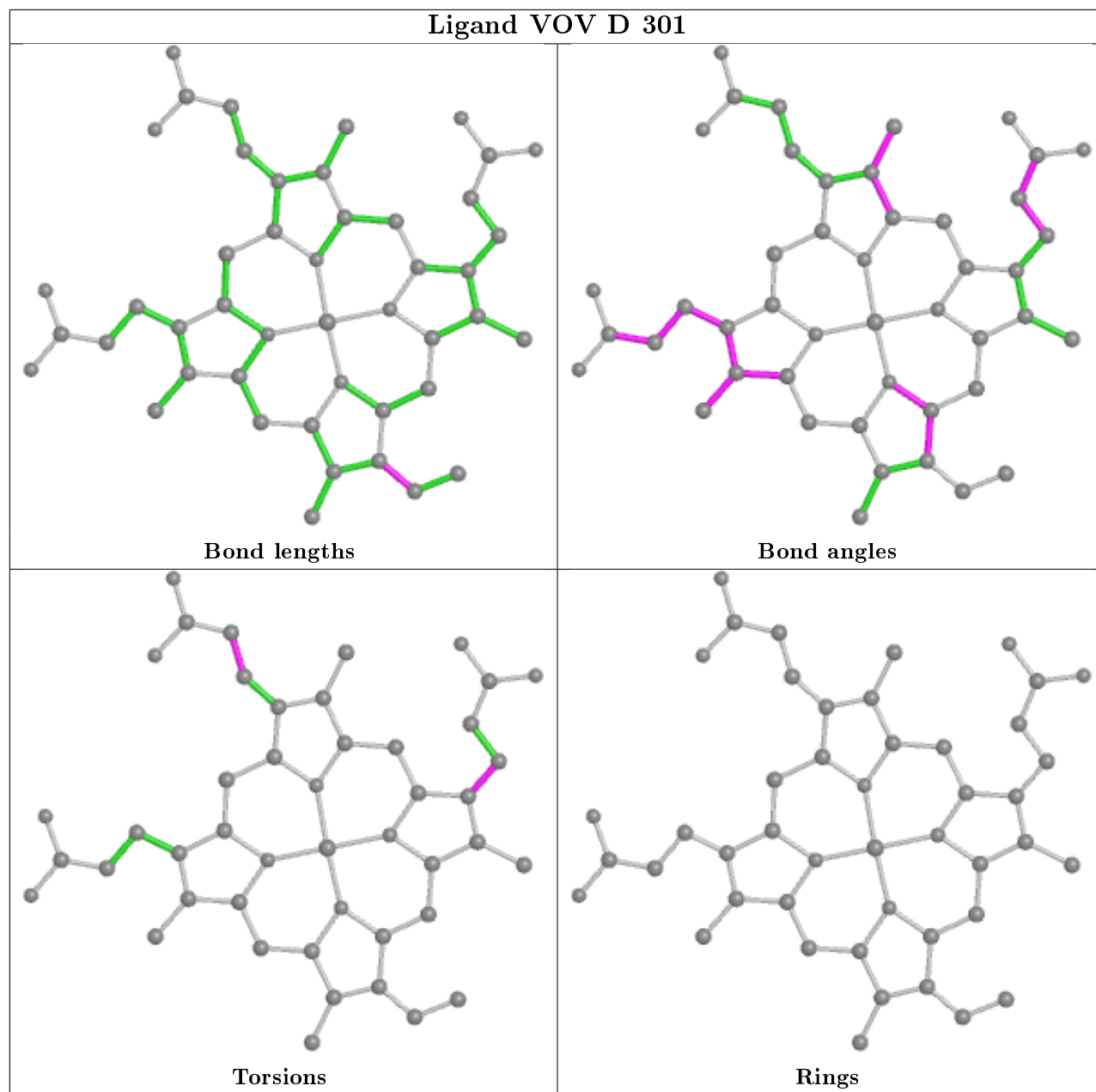
4 monomers are involved in 5 short contacts:

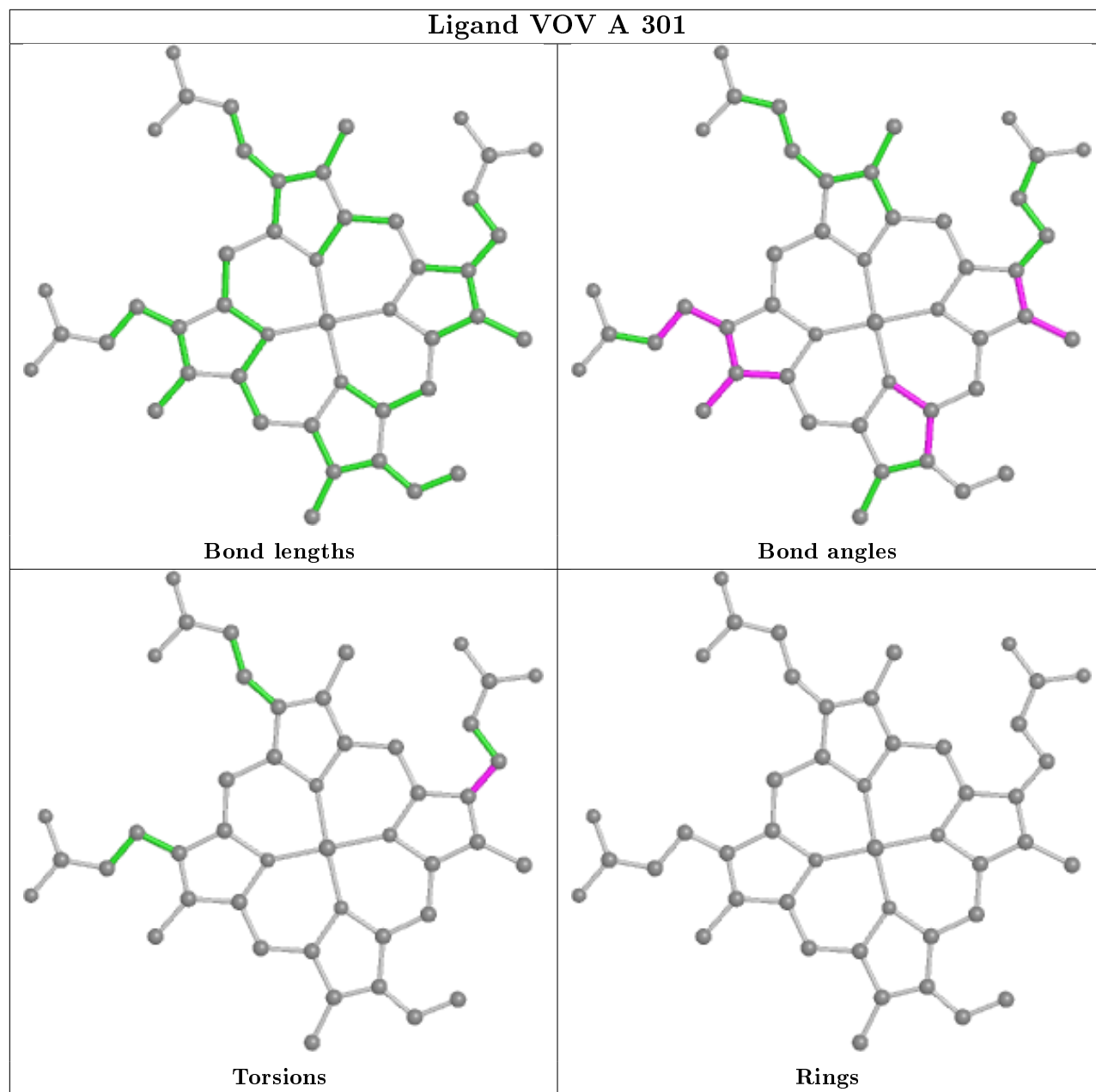
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	VOV	1	0
2	D	301	VOV	1	0
2	A	301	VOV	1	0
2	E	401	VOV	2	0

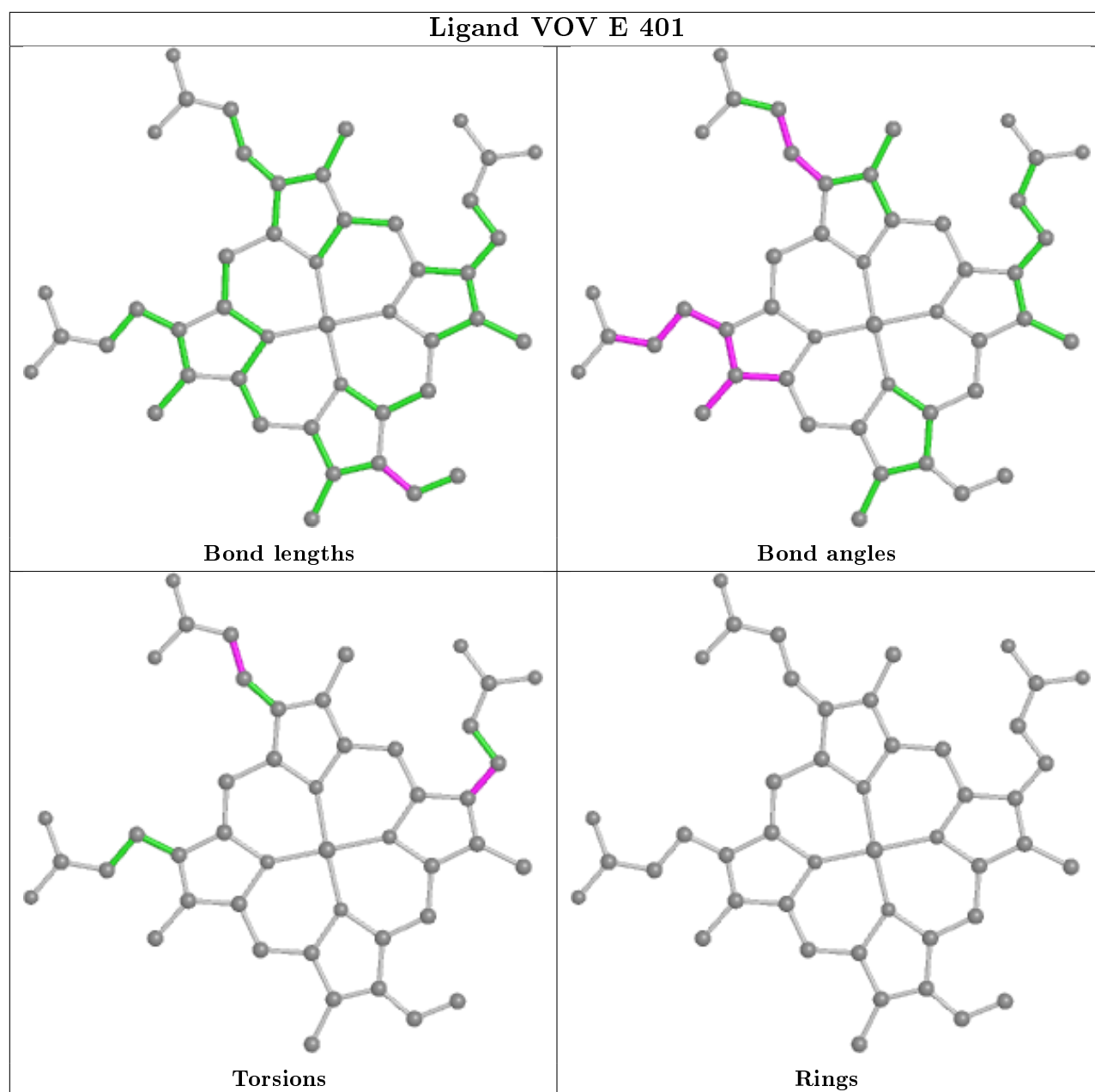
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/237 (97%)	0.30	5 (2%) 62 61	22, 32, 57, 95	0
1	B	231/237 (97%)	0.20	4 (1%) 70 70	24, 33, 59, 87	0
1	C	230/237 (97%)	0.30	10 (4%) 35 33	25, 36, 64, 86	0
1	D	228/237 (96%)	0.36	8 (3%) 44 42	27, 39, 64, 103	0
1	E	223/237 (94%)	0.47	14 (6%) 20 19	26, 39, 79, 119	0
All	All	1142/1185 (96%)	0.32	41 (3%) 42 41	22, 36, 64, 119	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	114	PHE	9.7
1	B	5	LEU	8.7
1	D	38	ALA	5.8
1	E	235	GLY	5.4
1	E	111	PRO	5.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

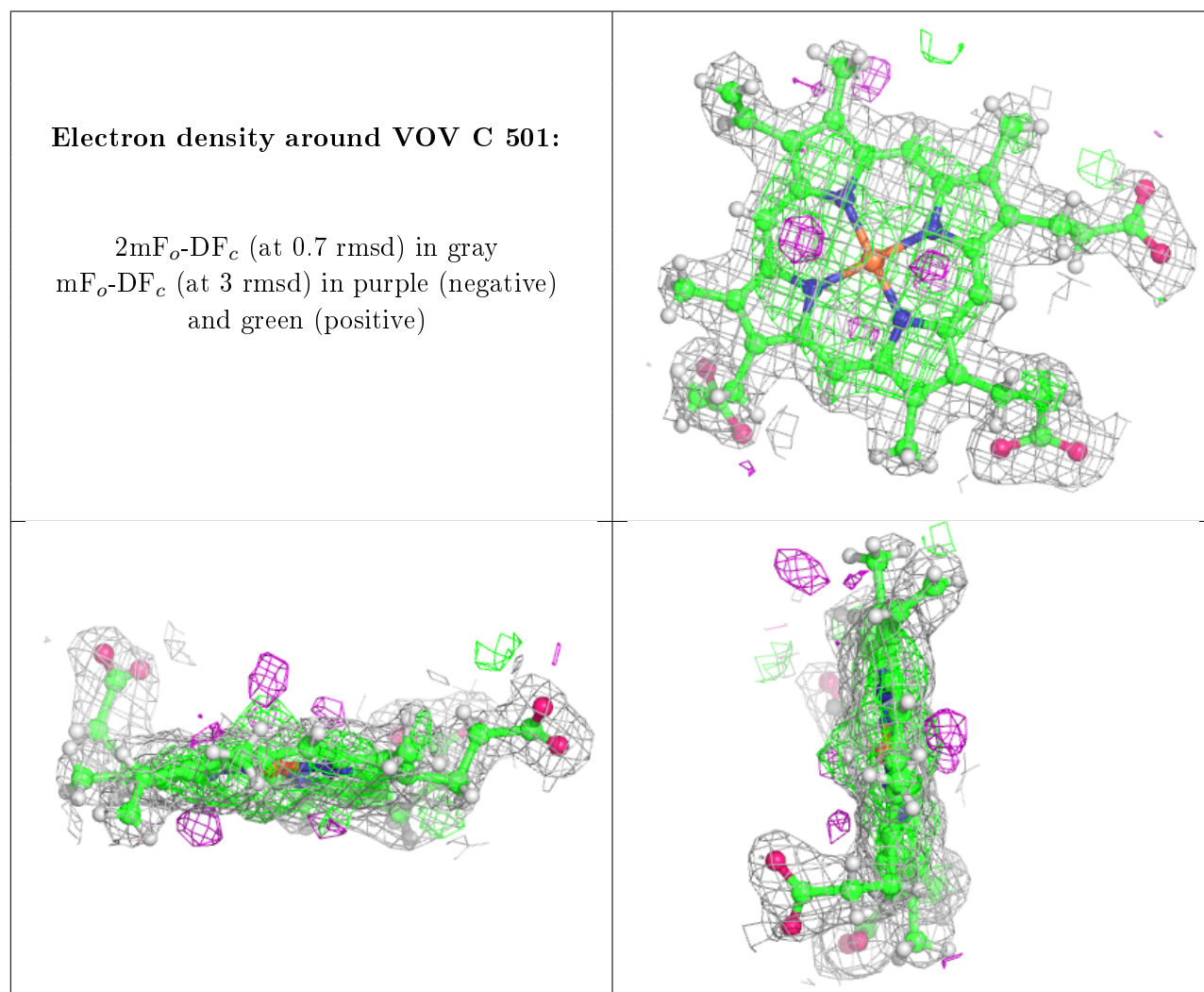
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

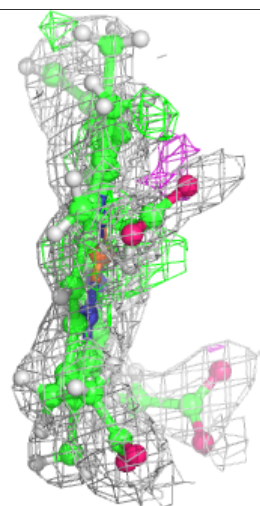
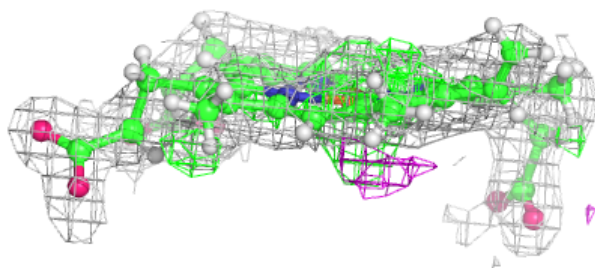
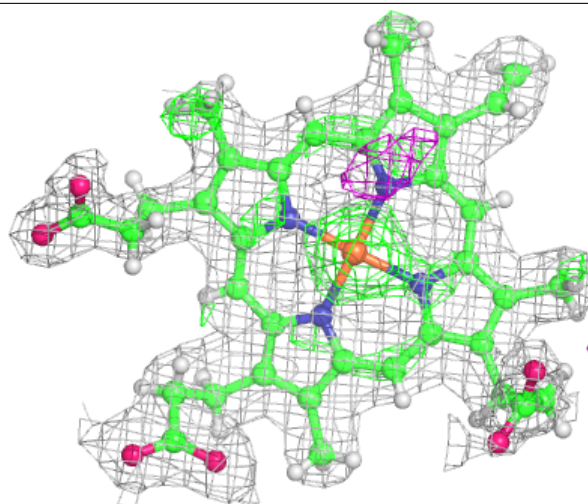
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	VOV	C	501	46/46	0.44	0.28	21,54,193,376	0
2	VOV	D	301	46/46	0.56	0.21	35,63,143,220	0
2	VOV	B	401	46/46	0.69	0.15	27,43,70,161	0
2	VOV	A	301	46/46	0.78	0.13	19,34,54,108	0
2	VOV	E	401	46/46	0.88	0.19	36,59,90,97	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



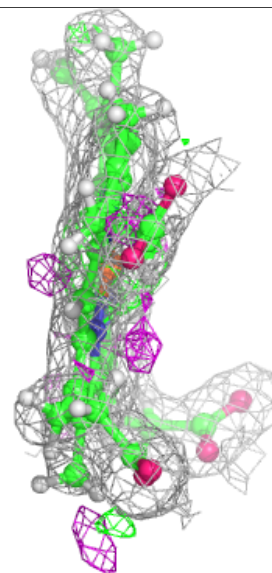
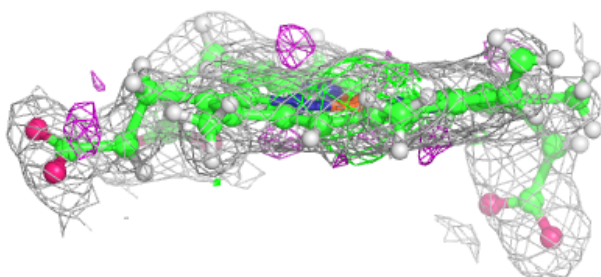
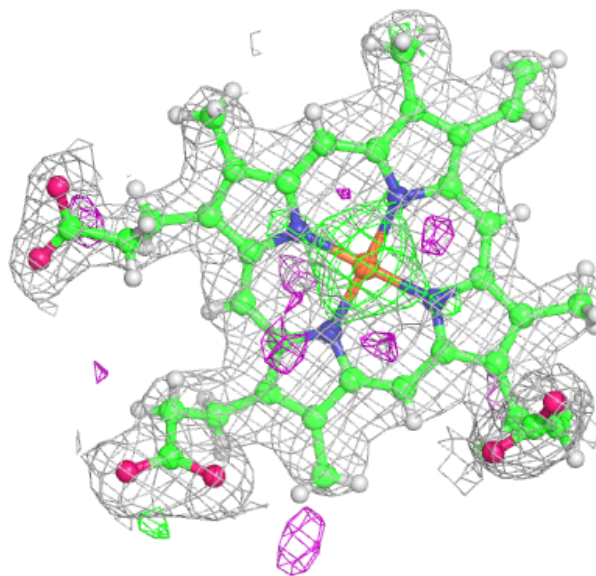
Electron density around VOV D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



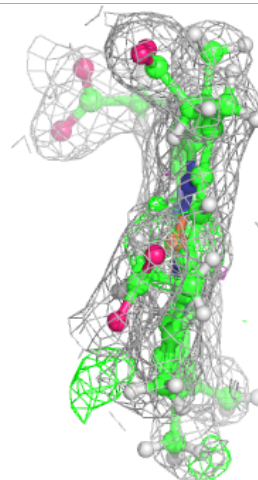
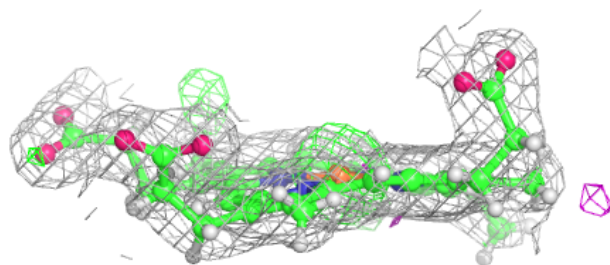
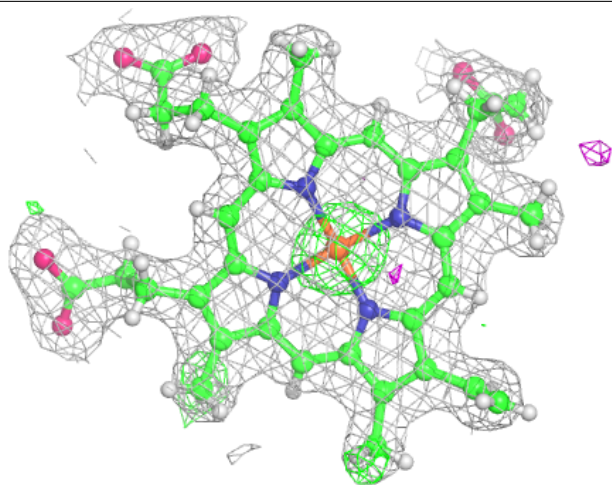
Electron density around VOV B 401:

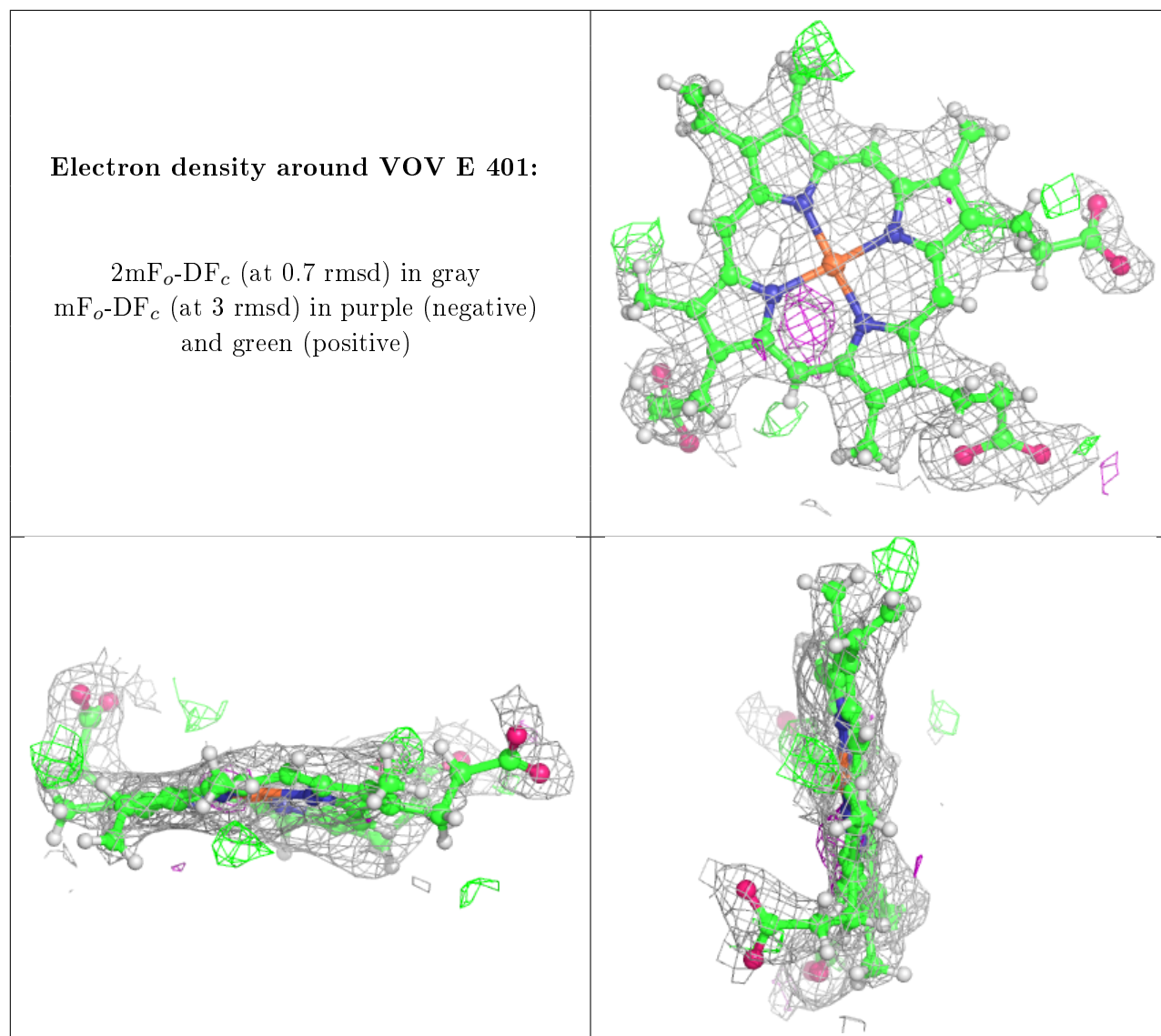
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VOV A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.